

Exhibit 1

Molecules To Go (NIH)

(Formerly known as Molecules R Us)

Request an image of a PDB file "the way you want it"!.

Instructions | PDB Search Form | NIH Home Page

Viewers provide interactive molecules, and require the appropriate helper application. Image selections provide static "gif" images, and Java options provide inline interactive displays.]

Viewing Molecule: Output Requested:

Parameters effect Static Image generation only:

Image to be generated by Rasimol (fast) ☒ or Raster3D (slow) ☐

Color by: (* => Rasmol only)

Rotations (0 - 360) degrees (for image only)

X-Axis: Y-Axis: Z_Axis:

First 100 lines from the PDB structure record... 1crl... Filesize = 109877

HEADER	HYDROLASE (CARBOXYLIC ESTERASE)	02-MAR-93	1CRL	1CRL	2
COMPND	LIPASE (E.C.3.1.1.3) (TRIACYLGLYCEROL HYDROLASE)			1CRL	3
SOURCE	FUNGUS (CANDIDA RUGOSA) (FORMERLY CYLINDRACEA)			1CRL	4
AUTHOR	P.GROCHULSKI,M.CYGLER			1CRL	5
REVDAT	1 31-JAN-94 1CRL 0			1CRL	6
JRNL	AUTH P.GROCHULSKI,Y.LI,J.D.SCHRAG,F.BOUTHILLIER,P.SMITH,			1CRL	7
JRNL	AUTH 2 D.HARRISON,B.RUBIN,M.CYGLER			1CRL	8
JRNL	TITL INSIGHTS INTO INTERFACIAL ACTIVATION FROM AN			1CRL	9
JRNL	TITL 2 'OPEN' STRUCTURE OF CANDIDA RUGOSA LIPASE			1CRL	10
JRNL	REF J.BIOL.CHEM.	V. 268 12843 1993		1CRL	11
JRNL	REFN ASTM JBCHA3 US ISSN 0021-9258		071	1CRL	12
REMARK	1			1CRL	13
REMARK	1 REFERENCE 1			1CRL	14
REMARK	1 AUTH Y.KAWAGUCHI,H.HONDA,J.TANIGUCHI-MORIMURA,S.IWASAKI			1CRL	15
REMARK	1 TITL THE CODON CUG IS READ AS SERINE IN AN ASPOROGENIC			1CRL	16
REMARK	1 TITL 2 YEAST CANDIDA CYLINDRACEA			1CRL	17
REMARK	1 REF NATURE	V. 341 164 1989		1CRL	18
REMARK	1 REFN ASTM NATUAS UK ISSN 0028-0836		006	1CRL	19
REMARK	2			1CRL	20
REMARK	2 RESOLUTION. 2.06 ANGSTROMS.			1CRL	21
REMARK	3			1CRL	22

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REMARK	3	REFINEMENT.			1CRL	23
REMARK	3	PROGRAM	X-FLOR		1CRL	24
REMARK	3	AUTHORS	BRUNGER		1CRL	25
REMARK	3	R VALUE	0.134		1CRL	26
REMARK	3	RMSD BOND DISTANCES	0.011	ANGSTROMS	1CRL	27
REMARK	3	RMSD BOND ANGLES	2.64	DEGREES	1CRL	28
REMARK	4				1CRL	29
REMARK	4	THREE N-ACETYLGLUCOSAMINE RESIDUES AT TWO SITES INCLUDED:			1CRL	30
REMARK	4	TWO N-LINKED RESIDUES AT ASN 351; ONE N-LINKED RESIDUE AT			1CRL	31
REMARK	4	ASN 314.			1CRL	32
SEQRES	1	534	ALA PRO THR ALA THR LEU ALA ASN GLY ASP THR ILE THR		1CRL	33
SEQRES	2	534	GLY LEU ASN ALA ILE ILE ASN GLU ALA PHE LEU GLY ILE		1CRL	34
SEQRES	3	534	PRO PHE ALA GLU PRO PRO VAL GLY ASN LEU ARG PHE LYS		1CRL	35
SEQRES	4	534	ASP PRO VAL PRO TYR SER GLY SER LEU ASP GLY GLN LYS		1CRL	36
SEQRES	5	534	PHE THR SER TYR GLY PRO SER CYS MET GLN GLN ASN PRO		1CRL	37
SEQRES	6	534	GLU GLY THR TYR GLU GLU ASN LEU PRO LYS ALA ALA LEU		1CRL	38
SEQRES	7	534	ASP LEU VAL MET GLN SER LYS VAL PHE GLU ALA VAL SER		1CRL	39
SEQRES	8	534	PRO SER SER GLU ASP CYS LEU THR ILE ASN VAL VAL ARG		1CRL	40
SEQRES	9	534	PRO PRO GLY THR LYS ALA GLY ALA ASN LEU PRO VAL MET		1CRL	41
SEQRES	10	534	LEU TRP ILE PHE GLY GLY GLY PHE GLU VAL GLY GLY THR		1CRL	42
SEQRES	11	534	SER THR PHE PRO PRO ALA GLN MET ILE THR LYS SER ILE		1CRL	43
SEQRES	12	534	ALA MET GLY LYS PRO ILE ILE HIS VAL SER VAL ASN TYR		1CRL	44
SEQRES	13	534	ARG VAL SER SER TRP GLY PHE LEU ALA GLY ASP GLU ILE		1CRL	45
SEQRES	14	534	LYS ALA GLU GLY SER ALA ASN ALA GLY LEU LYS ASP GLN		1CRL	46
SEQRES	15	534	ARG LEU GLY MET GLN TRP VAL ALA ASP ASN ILE ALA ALA		1CRL	47
SEQRES	16	534	PHE GLY GLY ASP PRO THR LYS VAL THR ILE PHE GLY GLU		1CRL	48
SEQRES	17	534	SER ALA GLY SER MET SER VAL MET CYS HIS ILE LEU TRP		1CRL	49
SEQRES	18	534	ASN ASP GLY ASP ASN THR TYR LYS GLY LYS PRO LEU PHE		1CRL	50
SEQRES	19	534	ARG ALA GLY ILE MET GLN SER GLY ALA MET VAL PRO SER		1CRL	51
SEQRES	20	534	ASP ALA VAL ASP GLY ILE TYR GLY ASN GLU ILE PHE ASP		1CRL	52
SEQRES	21	534	LEU LEU ALA SER ASN ALA GLY CYS GLY SER ALA SER ASP		1CRL	53
SEQRES	22	534	LYS LEU ALA CYS LEU ARG GLY VAL SER SER ASP THR LEU		1CRL	54
SEQRES	23	534	GLU ASP ALA THR ASN ASN THR PRO GLY PHE LEU ALA TYR		1CRL	55
SEQRES	24	534	SER SER LEU ARG LEU SER TYR LEU PRO ARG PRO ASP GLY		1CRL	56
SEQRES	25	534	VAL ASN ILE THR ASP SER MET TYR ALA LEU VAL ARG GLU		1CRL	57
SEQRES	26	534	GLY LYS TYR ALA ASN ILE PRO VAL ILE ILE GLY ASP GLN		1CRL	58
SEQRES	27	534	ASN ASP GLU GLY THR PHE PHE GLY THR SER SER LEU ASN		1CRL	59
SEQRES	28	534	VAL THR THR ASP ALA GLN ALA ARG GLU TYR PHE LYS GLN		1CRL	60
SEQRES	29	534	SER PHE VAL HIS ALA SER ASP ALA GLU ILE ASP THR LEU		1CRL	61
SEQRES	30	534	MET THR ALA TYR PRO GLY ASP ILE THR GLN GLY SER PRO		1CRL	62
SEQRES	31	534	PHE ASP THR GLY ILE LEU ASN ALA LEU THR PRO GLN PHE		1CRL	63
SEQRES	32	534	LYS ARG ILE SER ALA VAL LEU GLY ASP LEU GLY PHE THR		1CRL	64
SEQRES	33	534	LEU ALA ARG ARG TYR PHE LEU ASN HIS TYR THR GLY GLY		1CRL	65
SEQRES	34	534	THR LYS TYR SER PHE LEU SER LYS GLN LEU SER GLY LEU		1CRL	66
SEQRES	35	534	PRO VAL LEU GLY THR PHE HIS SER ASN ASP ILE VAL PHE		1CRL	67
SEQRES	36	534	GLN ASP TYR LEU LEU GLY SER GLY SER LEU ILE TYR ASN		1CRL	68
SEQRES	37	534	ASN ALA PHE ILE ALA PHE ALA THR ASP LEU ASP PRO ASN		1CRL	69
SEQRES	38	534	THR ALA GLY LEU LEU VAL LYS TRP PRO GLU TYR THR SER		1CRL	70
SEQRES	39	534	SER SER GLN SER GLY ASN ASN LEU MET MET ILE ASN ALA		1CRL	71
SEQRES	40	534	LEU GLY LEU TYR THR GLY LYS ASP ASN PHE ARG THR ALA		1CRL	72
SEQRES	41	534	GLY TYR ASP ALA LEU PHE SER ASN PRO PRO SER PHE PHE		1CRL	73
SEQRES	42	534	VAL		1CRL	74
FTNOTE	1				1CRL	75
FTNOTE	1	CIS PROLINE - PRO	390		1CRL	76
HET	NAG	990	14	N-ACETYL-D-GLUCOSAMINE	1CRL	77
HET	NAG	991	14	N-ACETYL-D-GLUCOSAMINE	1CRL	78
HET	NAG	994	14	N-ACETYL-D-GLUCOSAMINE	1CRL	79
FORMUL	2	NAG	3(C8 H15 N1 O6)		1CRL	80
FORMUL	3	HOH	*310(H2 O1)		1CRL	81
HELIX	1	H1 LEU	73 GLN	83 1 FLAP	1CRL	82

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HELIX	2	H2	ALA	136	MET	145	1										1CRL	83
HELIX	3	H3	ASP	167	GLU	172	1										1CRL	84
HELIX	4	H4	ALA	177	ASP	191	1										1CRL	85
HELIX	5	H5	ALA	210	LEU	220	1										1CRL	86
HELIX	6	H6	ILE	253	ALA	266	1										1CRL	87
HELIX	7	H7	LYS	274	ARG	279	1										1CRL	88
HELIX	8	H8	SER	283	THR	290	1										1CRL	89
HELIX	9	H9	ASP	318	ARG	324	1										1CRL	90
HELIX	10	H10	THR	343	THR	347	1										1CRL	91
HELIX	11	H11	ASP	355	SER	365	1										1CRL	92
HELIX	12	H12	ASP	371	ALA	380	1										1CRL	93
HELIX	13	H13	PHE	403	HIS	425	1										1CRL	94
HELIX	14	H14	ASP	452	GLN	456	1										1CRL	95
HELIX	15	H15	SER	464	ALA	475	1										1CRL	96
HELIX	16	H16	THR	519	LEU	525	1										1CRL	97
SHEET	1	BN	3	PRO	2	LEU	6	0									1CRL	98
SHEET	2	BN	3	ASP	10	GLY	14	-1	N	GLY	14	O	PRO	2			1CRL	99
SHEET	3	BN	3	GLY	50	PHE	53	1	N	PHE	53	O	THR	13			1CRL	100
SHEET	1	BC	11	LEU	15	ALA	17	0									1CRL	101
